Recovery of lithium from spent lithium-ion batteries using carbothermal reduction with spent coffee grounds: A parametric optimization using combined approach of response surface methodology and machine learning

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Suplementary data

S1 Machine learning models

S1.1 Decision tree regression

Decision Tree Regression is a supervised machine learning algorithm used for predicting continuous numerical values. It works by partitioning the data into subsets based on feature values, creating a tree-like structure where each node represents a decision rule, and the leaves represent the predicted output[1]. In a decision tree, the dataset is divided into subsets containing instances with similar values. The process begins at the root node, which splits into branches or sub-trees based on feature values, forming decision nodes. These decision nodes store information about the data features and rules for decision-making. As the tree progresses, it either further splits into

additional branches or provides an outcome, represented by leaf nodes, which indicate the decision or result derived from the previous splits[2].

S1.2 Random Forest regression (RFR)

Random Forest (RF) is a powerful ensemble learning method composed of multiple decision trees, capable of handling both regression and classification tasks. It is built using the bagging technique, where random samples and features are drawn with replacement from the original dataset to train each decision tree independently. At each node, only a randomly selected subset of features is considered for splitting, promoting diversity among the trees. This diversity reduces overfitting and enhances the model's generalization ability. During prediction, the RF algorithm aggregates the results from all decision trees, either by averaging for regression tasks or voting for classification tasks, to provide the final prediction[3].

S1.3 Extreme gradient boosting regression (XGBoost)

Extreme Gradient Boosting (XGBoost) is a powerful ensemble learning algorithm that constructs multiple decision trees to build a predictive model. Each successive decision tree is trained to correct the errors made by its predecessor, enhancing the model's overall accuracy. XGBoost achieves high predictive performance by incorporating a regularization technique that prevents overfitting, improving the model's generalization ability. This combination of error correction and regularization makes XGBoost highly efficient and effective for both regression and classification tasks[4].

S1.4 Explainable Artificial intelligence (XAI)

Explainable Artificial Intelligence (XAI) encompasses a range of methods and techniques within machine learning (ML) and artificial intelligence (AI) that aim to make the decision-making

processes and behaviors of models transparent and understandable[5]. XAI techniques provide insights into how models operate and generate predictions, enhancing their interpretability, trustworthiness, and usability. Among the XAI methods employed in this context are Shapley Additive Explanations (SHAP), Permutation Feature Importance (PFI) plots, and Partial Dependence Plots (PDP), all of which help to elucidate model behaviors and facilitate a deeper understanding of their outcomes. SHAP (Shapley Additive Explanations) provides a framework for attributing a quantitative "contribution" value to each feature in a predictive model, thereby elucidating the role of individual features in the model's decision-making process[6]. Partial dependence plots (PDP) technique used to assess the relationship between one or more features and the predicted outcome of a machine learning model, while controlling for the effects of other features. It is particularly valuable for understanding how changes in a feature impact the model's predictions, while keeping other features constant[7]. Similarly, permutation feature importance plots help visualize the impact of a feature on the model's output by evaluating the decrease in prediction accuracy when that feature is removed or shuffled[8].

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